

Cyclopropaneacetaldehyde, 2,2-dimethyl-3-(2-oxopropyl)-
26946-56-5 | DTXSID10447169

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 219 °C

Global applicability domain: Inside

Local applicability domain index: 6.29e-01

Confidence level: 7.77e-01

Nearest Neighbors from the Training Set

Image not found

Butyl 4-oxopentanoate

Measured: 238

Predicted: 228

Image not found

Diethyl cyclopropane-1,1-dicarboxylate

Measured: 216

Predicted: 222

Image not found

Ethyl 2,2-diethylacetoacetate

Measured: 216

Predicted: 219